Supplementary Material

## Enhanced Photocatalytic Performance of Stable Type –II PtSe<sub>2</sub>/GaSe Van der Waals Heterostructure

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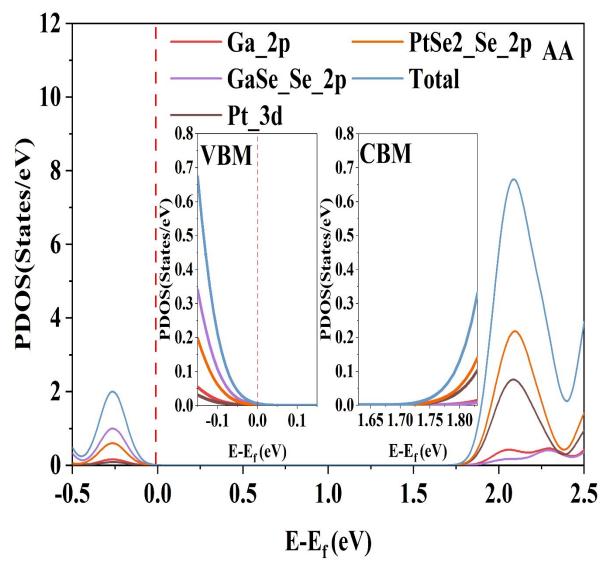


Fig. S1. Enlarged view of VBM and CBM of PDOS of vdwHS-AA

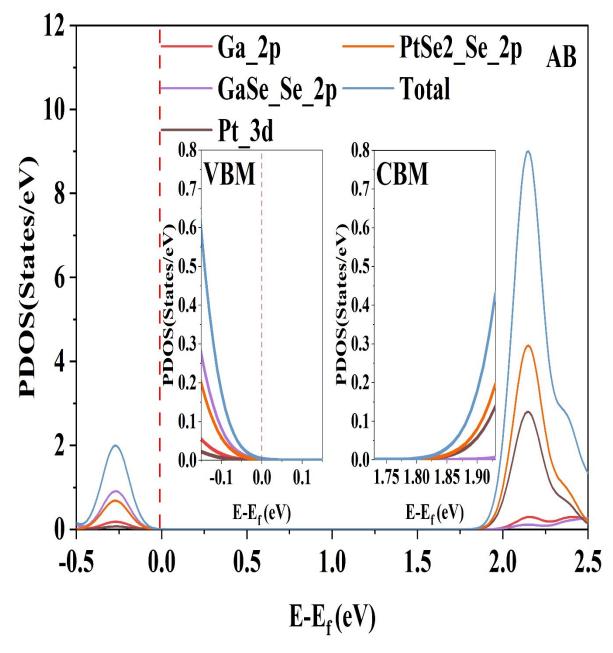


Fig. S2. Enlarged view of VBM and CBM of PDOS of vdwHS-AB

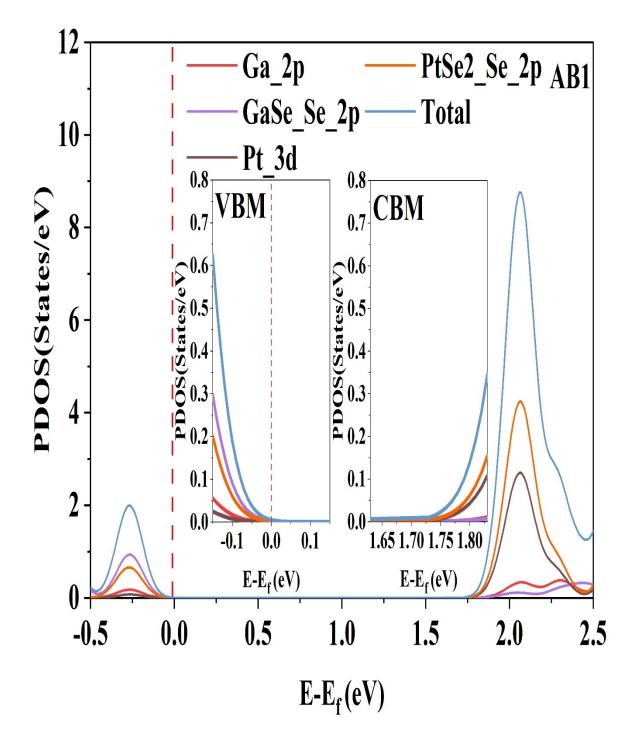


Fig. S3. Enlarged view of VBM and CBM of PDOS of vdwHS-AB1